



Slovak Society of Chemical Engineering
Institute of Chemical and Environmental Engineering
Slovak University of Technology in Bratislava

PROCEEDINGS

52nd International Conference of the Slovak Society of Chemical Engineering SSCHE 2026

Hotel SOREA TRIGAN
Štrbské Pleso, Slovakia
May 26 - 29, 2026

Editors: Assoc. prof. Mário Mihaľ

ISBN: 978-80-8208-177-3, EAN: 9788082081773

Published by the Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava in Slovak Chemistry Library for the Institute of Chemical and Environmental Engineering; Radlinského 9, 812 37 Bratislava, 2026

Árvai, C., Mika, L.: Phosphine-free Heck coupling reaction, in 1,4-pentanediol as an alternative biomass-derived medium, Editors: Mihaľ, M., In *52nd International Conference of the Slovak Society of Chemical Engineering SSCHE 2026*, Štrbské Pleso, Slovakia, 2026.

Phosphine-free Heck coupling reaction, in 1,4-pentanediol as an alternative biomass-derived medium

Csaba Árvai¹, László Tamás Mika¹

¹*Department of Chemical and Environmental Process Engineering, Budapest University of Technology and Economics, 1111 Budapest, Műegyetem rkp. 3, Hungary*

e-mail: csaba.arvai@edu.bme.hu

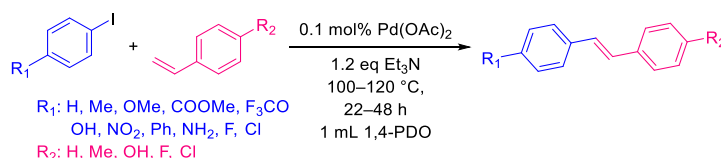
Keywords: Heck reaction, homogeneous catalysis, phosphine-free, green chemistry

In the field of multistep synthesis of biologically active compounds, transition metal-catalyzed cross-coupling reactions have become one of the most powerful tools for the construction of new carbon-carbon bonds. The Pd-catalyzed Heck reaction between an aryl halide and an alkene is a facile protocol to synthesize fine chemicals, including active pharmaceutical intermediates.¹ The reaction is usually carried out in conventional polar aprotic solvents, e.g., DMF or NMP, which are suspected carcinogens.

We have demonstrated that the biomass-originated 1,4-pentanediol (1,4-PDO) could be utilized as an alternative protic polar reaction medium for the homogeneous Ullmann-type C-N coupling reaction of aryl halides and primary or secondary amines.² Based on these results, our aim was to broaden the applicability of 1,4-PDO with the Heck reaction.

It was shown that 1,4-PDO can be used as a medium for phosphine-free Pd-catalyzed synthesis of several stilbene derivatives. Cooling the reaction mixture to room temperature resulted in the product precipitating as brownish crystals, facilitating product isolation.

In our presentation, we will discuss the effects of various reaction parameters (e.g., temperature, catalyst precursor, base, and para-substituent derivatives of the substrates) on system activity (Scheme 1), the general low E-factor isolation method, and the parallel solvent-catalyst recycling.³



Scheme 1 Pd-catalyzed Heck-coupling of iodobenzene and its para-substituted derivatives with styrene and its para-substituted derivatives

- ¹ G. Rossino, G. Marrubini, M. Brindisi, M. Granje, P. Linciano, D. Rossi, S. Collina, "A green Heck reaction protocol towards trisubstituted alkenes, versatile pharmaceutical intermediates" *Front. Chem.* **2024**, *12*, 1431382.
- ² C. Árvai, L. T. Mika, "Application of 1,4-pentanediol as a renewable solvent for copper-catalyzed Ullmann-type coupling reactions." *J. Organomet. Chem.* **2024**, *1005*, 122976.
- ³ C. Árvai, L. T. Mika, "1,4-Pentanediol as an Alternative Biomass-Derived Medium for the Phosphine-Free Heck Coupling Reactions." *ChemSusChem* **2026** *in press* <https://doi.org/10.1002/cssc.70666>